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SHORT COMMUNICATION

Rotational Isomerism in Fluorinated Compounds:

1,3-Difluoro-2-propanol

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Rotational isomerism has been shown to exist in 1,3-difluoro-2-propanone [1,2], which exists as two conformers which were tentatively identified as the gauche-gauche and cis-gauche. That compound is structurally similar to 1,3-difluoro-2-propanol, so the conformational behavior of the alcohol is of interest for comparison with the ketone.

The liquid-state infrared spectrum of the alcohol shows the expected broad O-H stretching band, centered at about 3420 cm^{-1} , due to hydrogen-bonded species, but there is also a weaker band at 3587 cm^{-1} that is due to the unassociated O-H stretch, so this alcohol is not completely associated in the neat liquid.

Infrared spectra were also obtained for several solutions of the alcohol in CCl_4 and CS_2 solutions in the concentration range 10% to ca. 0.1%. Several changes take place in the spectrum as the solute concentration is decreased. These changes are shown in Fig. 1 for the O-H stretch region. As expected, the intensity of the broad band due to the associated species decreases with increasing dilution, as the alcohol becomes less associated. However, there are two monomer O-H bands, at 3601 and 3622 cm^{-1} , that can only be due to the presence of two rotational isomers. The intensity of the 3622 cm^{-1} band of this pair increases at the expense of the other one as dilution increases. Therefore, the 3622 cm^{-1} band can be assigned to the less polar conformer, since this conformer

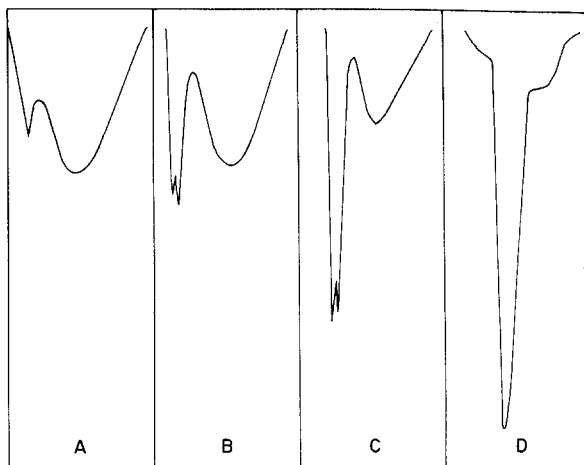


Fig. 1. Infrared spectra of $\text{CH}_2\text{FCHOHCH}_2\text{F}$ in the O-H stretch region. A, neat; B, 5% in CCl_4 ; C, 1% in CCl_4 ; D, ca. 0.1% in CCl_4 .

will be stabilized relative to the more polar conformer in nonpolar solvents.

The C-O-H bending and -OH torsional bands also change with increasing dilution because of the decreasing association. The C-O-H bend can be assigned to bands at ca. 1300 cm^{-1} (associated) and 1220 cm^{-1} (monomer) from their behavior in solution. There are two bands in the $600\text{--}700\text{ cm}^{-1}$ region in the liquid state spectrum, at 649 and 671 cm^{-1} . The intensity of the 671 cm^{-1} band decreases with increasing dilution, and this band is absent in the vapor-state spectrum, so it can be assigned to the associated -OH torsion. The monomer torsional band lies below the region investigated.

The last major spectral change that occurs with increasing dilution concerns the pair of strong bands observed at 1119 and 1140 cm^{-1} in the neat liquid. As dilution increases, the intensity of the 1119 cm^{-1} band increases at the expense of the 1140 cm^{-1} band. This behavior shows that the 1119 cm^{-1} band is due to the less polar conformer and the 1140 cm^{-1} band is due to the more polar conformer. This conclusion is verified by the almost complete absence of the 1140 cm^{-1} band in the vapor-state spectrum. This band is barely observed as a very weak shoulder, so the more polar conformer is almost

absent in the vapor state. 1,3-Difluoro-2-propanone showed the same behavior [1]. The less polar conformer is undoubtedly stabilized by an internal hydrogen bond between the hydroxyl hydrogen and one of the fluorine atoms, in the same way as 2-fluoroethanol [3-5].

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